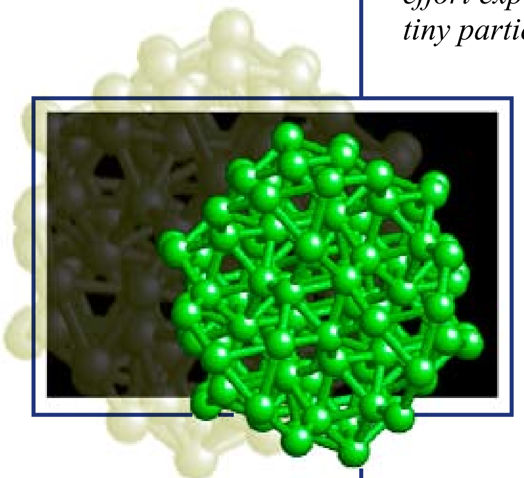
NLCF Explores the Potential of Burning Metal as the Fuel of the Future

Visions of a hopeful energy future typically feature hydrogen fuel cells powering automobiles and providing electricity. The National Leadership Computing Facility (NLCF) at Oak Ridge National Laboratory (ORNL) is a key part of a research effort exploring an alternative future—engines powered by the combustion of tiny particles of metal.



Boron nanoparticle structure derived from calculations.

A group of chemists and engineers at ORNL (Bobby Sumpter, David Beach, and Solomon Labinov) are conducting laboratory experiments (David Beach) and large-scale first-principles calculations on the NLCF computers to explore the potential of metallic nanoparticles as a fuel. (Their work was featured on the cover of the October 22, 2005, *New Scientist* magazine.) Like hydrogen, many metals are potent energy carriers and release almost no polluting emissions when they burn. They contain more energy per volume unit than hydrogen and are much easier to store and transport. In addition, oxidized metals can be converted back to usable fuel by chemical reduction. (For example, iron oxides can be reduced to iron by heating the oxidized metal in a stream of hydrogen gas.) However, much research remains to assess the viability of nanoparticles as a fuel and optimize the size and structure of the particles.

The initial stages of this project were carried out using iron nanoparticles, and laboratory experiments were carried out in concert with computer simulations and theoretical studies. As the focus of the project shifts to boron and aluminum, which are better candidates for transportation fuels, experimentation will be less straightforward and computation will be more critical for success.

The metallic nanofuels project poses several theoretical, computational, and computational challenges that demand computing capability at the level offered by the NLCF, according to Bobby Sumpter, who carries out the first-principles modeling of nanoparticle combustion. "This is a true grand challenge for computation. This project has enormous theory, computation, and simulation ramifications, which will be a crucial part of defining its success."

The project team is now using the NLCF computers to determine an equilibrium structure for a cluster of boron atoms, a building point for further computation. After that work is completed, the project team plans to use the NLCF machines to analyze three essential issues:

- The melting points of boron nanoparticles as a function of particle size and pressure must be determined to calculate the optimal size of boron particles in the nanofuel cluster (The size range of the particles in a cluster is critical; a small percentage of particles outside the range might cause the cluster to melt and loose its original nanostructure, which is critical for regeneration.) It would be difficult to make these determinations experimentally because of the problems associated with generating metallic nanoparticles of uniform size and with manipulating and characterizing such minute amounts of material physically.

- The thickness of the oxide layer needed to stabilize the fuel must be calculated. Too thin a layer could allow spontaneous combustion of the fuel; too thick a layer will require too much energy to ignite the fuel. This is an enormous set of calculations, but it is needed to facilitate the experimental preparation and validation.
- A computational study is needed to examine whether it is possible to adsorb enough oxygen onto the surface of a nanoparticle to carry out complete combustion of the nanoparticle (for environments without abundant oxygen). It would not be time - or cost-effective to explore the range of possibilities through experimentation alone.

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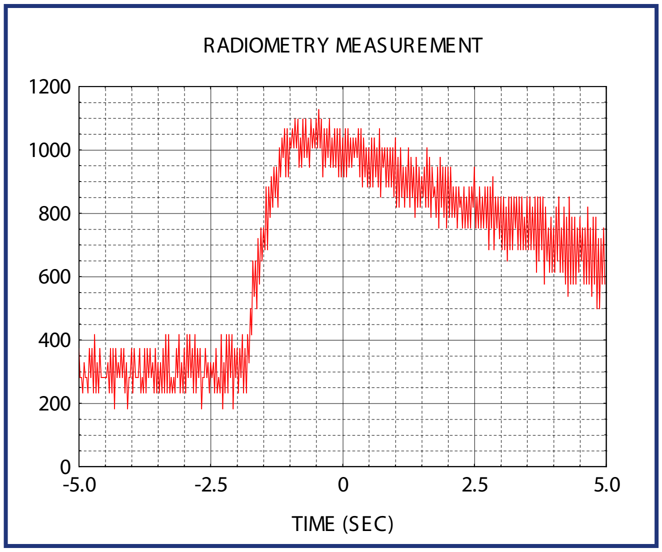

Experimentally determined combustion temperature for an engineered iron cluster composed of 50-nm iron particles.